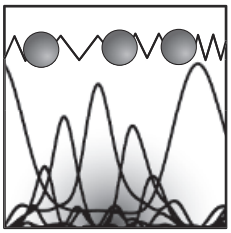

Project 10
The Fermi–Pasta–Ulam–Tsingou Problem

At the beginning of this book we discussed a simple problem of a harmonic oscillator (Project 3), which we then expanded into a problem of coupled oscillators (Project 9). Throughout this project, however, we considered only linear interactions between the oscillators. We also covered methods of solving differential equations and their use in initial value problems (IVP). In this project, we consider a chain of many bodies interacting with each other through a non-linear force. In literature, it is known as the Fermi-Pasta–Ulam–Tsingou problem. The analysis of the physical properties of such a system leads to unexpected observations. First, we see a spontaneous generation of oscillation modes of higher frequencies (i.e. frequency multiplication). Second, from a seemingly chaotic motion an order emerges, which includes a periodicity of that motion in time. This has been possible through the numerical methods described in this book.

10.1 Problem: Dynamics of a One-Dimensional Chain of Interacting Point Masses

Let us consider a chain of interacting point masses m (Figure 10.1). Their equilibrium positions are expressed by a vector of coordinates on the X axis, $\boldsymbol{x} = (\ldots, x^o_{i-1}, x^o_i, x^o_{i+1}, \ldots)$. Let's also assume that the distance between neighbouring masses is constant $x_i - x_{i-1} = a$, and call it the lattice constant a. The masses are allowed to move along the X axis, which is expressed by a time-dependent displacement vector $\boldsymbol{y} =$

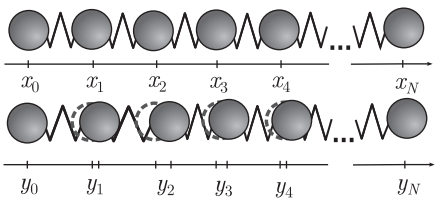

Figure 10.1 Chain of oscillating masses

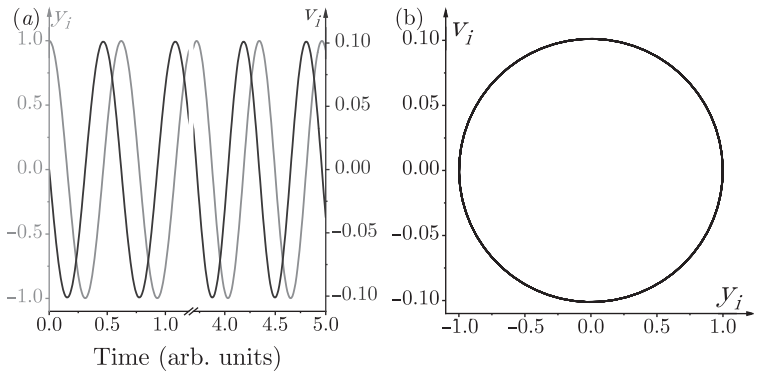

Figure 10.2 Coordinates of the central mass in a harmonic motion $N = 32$, $a = 1$, $m = 1$, $\alpha = 1$, $\beta = 0$: (a) time dependent, (b) in the form of phase diagram

$(\ldots, y_{i-1}, y_i, y_{i+1}, \ldots)$, where $y_i = x_i - x_i^o$ and x_i is the time-dependent position of the mass.

Newton's equations of motion for the i-th mass

$$\frac{\partial^2 y_i}{\partial t^2} = F(y_{i+1} - y_i) - F(y_i - y_{i-1}). \tag{10.1.1}$$

The expression for the force (right side of the equation) suggests that only the nearest-neighbour interactions are considered, and that the force depends on the difference in the displacements (a relative displacement). Let's start from a linear dependence of the force on the relative displacement $F(y_{i+i} - y_i) = \alpha(y_{i+1} - y_i)$, which simplifies Eq.10.1.1 to

$$\frac{\partial^2 y_i}{\partial t^2} = \alpha(y_{i+1} + y_{i-1} - 2y_i). \tag{10.1.2}$$

With this form of the equation, we expect that locally the oscillations are harmonic (Figure 10.2), and the motion of two different masses can differ only by a phase factor (due to their periodic symmetry). Taking those two factors into consideration, we can postulate a solution

$$y_i = Ae^{i(\omega t - kx_i)}. \tag{10.1.3}$$

It is a function that describes a wave, where $\omega = \frac{2\pi}{T}$ is the angular frequency (T is the period of oscillation) and $k = \frac{2\pi}{\lambda}$ is the wavenumber (λ is the wavelength, equal to or greater than the minimum wavelength allowed in the system, $\lambda \geq 2a$). A substitution of Eq. 10.1.3 in Eq. 10.1.2 leads to an expression for the dispersion relation, a detailed derivation of which can be found in the supplementary material (Appendix A.4)

$$\omega(k) = \sqrt{\frac{2\alpha}{m}[1 - \cos(ka)]}, \tag{10.1.4}$$

with k varying between $-\frac{\pi}{2}$ and $\frac{\pi}{2}$ (first Brillouin Zone). If we limit the length of the chain, assuming that masses x_0 and x_N are immobilised, that is $y_0 = y_N = 0$, then only standing waves (or their superpositions) can be excited in the chain, for which Eq. 10.1.4 can be factorised into spatial temporal components (see Project 6)

$$y = A\cos(\omega t)\sin(kx). \tag{10.1.5}$$

The left boundary condition for the spatial part is automatically fulfilled, due to the choice of the sine function. In order to fulfil the right boundary condition, the following condition must be fulfilled

$$y_N = A\sin(kaN) = A\sin(kL) = 0,$$

where $L = aN$ is the total length of the chain. This leads to a discretisation of allowed wave modes (normal modes)

$$k^n L = n\pi,$$

which means that the wavevector can only have discrete values

$$k^n = \frac{n\pi}{L},$$

with $n = 1, \ldots, N-1$.

For a given chain of length L, the longest normal mode is always $\lambda_{\max} = 2L$, while the shortest is the above-mentioned shortest wavelength $\lambda_{\min} = \frac{2L}{N-1}$. This means that the set of allowed modes is not only discrete but also finite, because we can have at most $N-1$ normal modes. The set can be expressed as

$$\{\boldsymbol{y}^{n0} = A^n \sin(k^n x_1^o), \ldots, \sin(k^n x_{N-1}^o)), \quad n = 1, \ldots, (N-1)\}. \tag{10.1.6}$$

In the above equation, A^n is the amplitude of the n-th mode and the upper index 0 indicates $t = 0$ in Eq. (10.1.5). The normal modes make up an orthonormal base in $N-1$ dimensional space, which can be normalised by an appropriate choice of the amplitudes A^n, so that the following relation is fulfilled

$$\boldsymbol{y}^{i0} \cdot \boldsymbol{y}^{j0} = \delta_{ij}.$$

An inclusion of the time-dependent part results in

$$\boldsymbol{y}^n(t) = \boldsymbol{y}^{n0}\cos(\omega^n t), \tag{10.1.7}$$

where $\omega^n = \omega(k^n)$ is the angular frequency associated with the n-th mode, given by the dispersion relation (10.1.4).

We can now derive the vector of velocities in the n-th mode as a time derivative of the displacement vector (10.1.7)

$$\boldsymbol{v}^n(t) = -\boldsymbol{y}^{n0}\omega^n \sin(\omega^n t). \tag{10.1.8}$$

This allowed us to find the trajectory in a multidimensional phase space for each mode.

Let's include a non-linear, second-order interaction

$$F(y_{i+1} - y_i) = \alpha(y_{i+1} - y_i) + \beta(y_{i+1} - y_i)^2. \tag{10.1.9}$$

We assume that the initial state of the chain is the first normal mode from the y^{n0} set, with an amplitude A

$$\boldsymbol{y}(t=0) = \frac{A}{A^1}\bar{y}^{10} = A(\sin(k^1 x_1^o), \ldots, \sin(k^1 x_{N-1}^o)), \tag{10.1.10}$$

with zero initial velocities $\bar{v}(t=0) = (0, \ldots, 0)$.

The energy of such a chain is therefore initially only the potential energy of the interaction

$$E = \sum_{i=1}^{N} U(y_i^{1o} - y_{i-1}^{1o}), \tag{10.1.11}$$

where $U(y) = -(\frac{1}{2}\alpha y^2 + \frac{1}{3}\beta y^3)$, and should be conserved throughout the entire motion.

Therefore, we have a system of differential equations (10.1.1) to solve. We use numerical methods, similarly as in the pendulum (Project 3), and coupled oscillator projects (Project 9). As a result, we obtain a time evolution of the trajectories in a multidimensional phase space of the coordinate and velocity vectors $\boldsymbol{y}(t)$ and $\boldsymbol{v}(t)$. The observation of the time evolution of a trajectory of a chosen mass (which can be done by plotting velocity as a function of position, see Figure 10.3) leads to

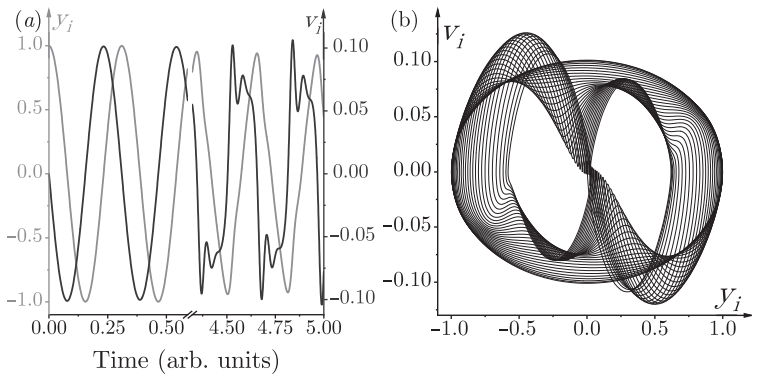

Figure 10.3 Coordinates of the central mass in a non-harmonic motion $N = 32$, $a = 1$, $m = 1$, $\alpha = 1$, $\beta = 0.25$: (a) time dependent, (b) phase diagram

the conclusion that the motion is chaotic. However, a certain order can be observed within that chaos. To do this observation, let us project the time-dependent displacements vector into fundamental modes, which, as we can remember, form an orthonormal basis

$$\boldsymbol{y}(t) = \sum_{n=1}^{N-1} a^n(t)\hat{y}^{n0}. \tag{10.1.12}$$

The coefficients a^n are projections of the state of the system onto the fundamental modes

$$a^n(t) = \boldsymbol{y}(t) \cdot \hat{y}^{n0}. \tag{10.1.13}$$

A similar representation can be performed for the velocity (using the same basis)

$$\boldsymbol{v}(t) = \sum_{n=1}^{N-1} b^n(t)\hat{y}^{n0}, \tag{10.1.14}$$

where the coefficients b^n are

$$b^n(t) = \boldsymbol{v}(t) \cdot \hat{y}^{n0}. \tag{10.1.15}$$

By doing this, we moved the entire time dependence to the coefficients $\{a^n(t)\}$ and $\{b^n(t)\}$. Now, instead of tracking the position and velocity of a given mass, we can observe the evolution of the coefficients, where the trajectories appear to be quite regular (see Figure 10.4). Let's focus on the energy and its flow through the modes (Figure 10.5). The energy associated with a given mode n is the sum of

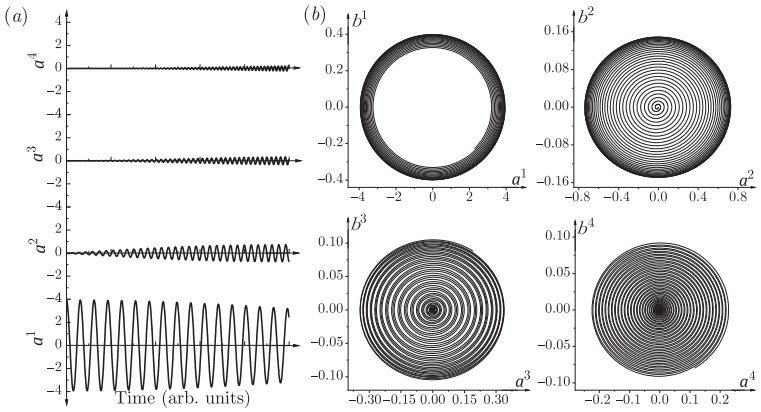

Figure 10.4 Coefficients $a^i(t)$ and $b^i(t)$ for i=1, 2, 3, and 4 respectively, for the case as in Figure 10.3: (a) time dependent, (b) phase diagram

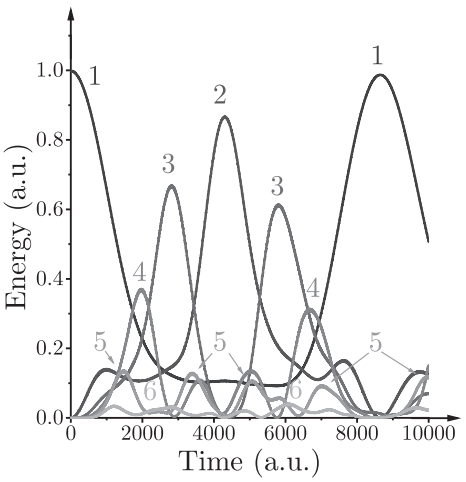

Figure 10.5 Solution for $N = 32$, $\alpha = 1$ and $\beta = 1/4$, originally obtained by Enrico Fermi, John Pasta, Stanisław Ulam and Mary Tsingou in 1955 (The numbers above the curves denote modes.)

potential and kinetic energies

$$E^n(t) = \sum_{i=1}^{N} U(y_i^n - y_{i-1}^n) + \sum_{i=1}^{N-1} \frac{1}{2} m v_i^{n2}, \tag{10.1.16}$$

where the upper index is the mode number, and the lower index indicates the mass. We can also write the condition for energy conservation

$$\sum_{n=1}^{N-1} E^n(t) = \text{const} = \sum_{i=1}^{N} U(y_i^{10} - y_{i-1}^{10}). \tag{10.1.17}$$

The computational procedure is now as follows. We solve the system of coupled differential equations (IVP – initial value problem), using one of the methods described in Project 3, while similarly to the coupled oscillators (Project 9), we recommend the Runge–Kutta method. For every fixed number of time steps (which speeds up the algorithm), we calculate the coefficients $a^n(t)$ and $b^n(t)$ from the dot products (10.1.13) and (10.1.15), which allow us to calculate the energies $E^n(t)$ with the use of (10.1.12), (10.1.14), and (10.1.16). That way we can obtain the time dependence of these quantities. The total energy as a function of time (which should be constant) will serve as a criterion for a proper choice of the time step (the optimal time step is the biggest time step that still keeps the conservation of energy).

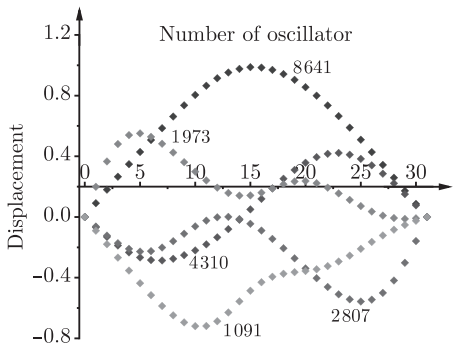

Figure 10.6 Displacements of masses at different instances of time

10.2 Exercises

1. Before proceeding to each of the exercises where the parameters of the system are changed (the number of masses, coefficients of interactions), a convergence test with respect to the time step h should be performed. The criterion for a proper choice is the conservation of energy with respect to time. In order to practice the procedure, try to find the largest h for which the energy is conserved. Use the amplitude distribution for the first mode as initial positions (and zero velocities).
2. For the system from the previous exercise perform a simulation of motion. For a few chosen time instances plot the positions of the mass (see Figure 10.6). Based on that plot, choose one relatively complicated state of positions, and knowing the coefficients $a^n(t)$ plot in a single figure $\boldsymbol{y}(t)$, and its component $\{a^n(t)\hat{y}^{n0}\}$.
3. For a chosen system plot the time dependence and phase portraits of position and velocity of a chosen mass and $a^n(t)$ and $b^n(t)$ coefficients (see Figures 10.3 and 10.4). Repeat the exercise for three cases: linear interaction only, non-linear interaction only, and both interactions at the same time.
4. The most interesting aspect of the FPUT problem is the frequency multiplication and energy transfer between modes. The first one was present in Exercise 2 already, where the initial condition was a fundamental mode; higher-order modes appear after some time. Now we investigate the time dependence of the energy components.
   For a given system, plot the total energy $E(t)$ and energy components $\{E^n(t)\}$ as a function of time (see Figure 10.5). Repeat the exercise for three cases: linear interaction only, non-linear interaction only, and both interactions at the same time.

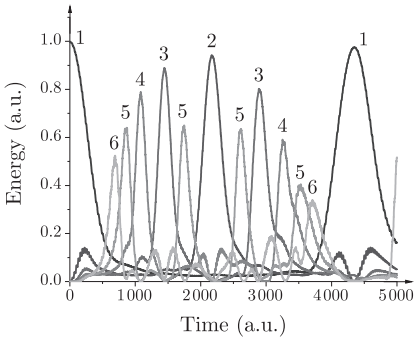

Figure 10.7 Results for $N = 32$, $a = 1$, $m = 1$, $\alpha = 1$, $\beta = 1$. Larger magnitude of the β parameter results in the emergence of higher-order modes

5. Investigate how the non-linear interaction parameter influences the speed of higher-order mode generation, their number and amplitude (see Figure 10.7). Suggest an appropriate numerical experiment. Add a third-order interaction and check its influence on a chosen example (without a detailed analysis).

A.3 Wilberforce's Pendulum

Lagrangian of Wilberforce's pendulum has the form

$$L = \frac{1}{2}m\dot{z}^2 + \frac{1}{2}I\dot{\theta}^2 - \frac{1}{2}kz^2 - \frac{1}{2}\delta\theta^2 - \frac{1}{2}\epsilon z\theta. \tag{A.3.1}$$

We use Euler–Lagrange equation

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0, \tag{A.3.2}$$

to obtain equations of motion

$$\frac{d}{dt}(m\dot{z}) + kz + \frac{1}{2}\epsilon\theta = 0, \tag{A.3.3}$$

$$\frac{d}{dt}\left(I\dot{\theta}\right) + \delta\theta + \frac{1}{2}\epsilon z = 0, \tag{A.3.4}$$

$$m\ddot{z} + kz + \frac{1}{2}\epsilon\theta = 0, \tag{A.3.5}$$

$$I\ddot{\theta} + k\theta + \frac{1}{2}\epsilon z. \tag{A.3.6}$$

A.4 Dispersion Relation for FPU Problem

To receive dispersion relation for an infinite chain of interacting masses (Project 10) we start with Newton's equation for i-th mass

$$m\frac{\partial^2 y_i}{\partial t^2} = \alpha(y_{i+1} + y_{i-1} - 2y_i), \tag{A.4.1}$$

in which we introduce a solution in a waveform

$$y_i = Ae^{i(\omega t - kx_i)}, \tag{A.4.2}$$

This substitution leads to

$$-m\omega^2 y_i = \alpha(y_{i+1} + y_{i-1} - 2y_i). \tag{A.4.3}$$

We want to determine ω, so we note that

$$\frac{y_{i+1}}{y_i} = \frac{Ae^{i(\omega t - kx_{i+1})}}{Ae^{i(\omega t - kx_i)}} = e^{-ik(x_{i+1} - x_i)} = e^{-ika}, \tag{A.4.4}$$

where we use lattice constant a as a distance between two masses in equilibrium points.

We use this result when dividing the previous equation by y_i

$$-m\omega^2 = \alpha(e^{-ika} + e^{ika} - 2) = \alpha(2\cos(ka) - 2) = 2\alpha[\cos(ka) - 1], \tag{A.4.5}$$

which leads to the dispersion relation

$$\omega(k) = \sqrt{\frac{2\alpha}{m}[1 - \cos(ka)]}. \tag{A.4.6}$$

A.5 Equivalence of Variational Principle and Poisson's Equation in Electrostatics

To prove the equivalence of the Poisson's differential equation and the variational principle, let us consider the functional

$$F[\phi] = \int_V d^3\mathbf{r}\left[\frac{1}{2}(\nabla\phi(\mathbf{r}))^2 - 4\pi\rho(\mathbf{r})\phi(\mathbf{r})\right]. \tag{A.5.1}$$

and its change with respect to potential variation $\delta\phi(\mathbf{r})$, which, according to the variational principle, should be zero

$$\delta F = \int_V d^3\mathbf{r}\left[\nabla\phi(\mathbf{r})\cdot\nabla\delta\phi(\mathbf{r}) - 4\pi\rho(\mathbf{r})\delta\phi(\mathbf{r})\right]. \tag{A.5.2}$$

Using the identity

$$\nabla\cdot(a\mathbf{b}) = (\nabla a)\cdot\mathbf{b} + a(\nabla\cdot\mathbf{b}), \tag{A.5.3}$$

in which we substitute $a = \delta\phi(\mathbf{r})$ and $\mathbf{b} = \nabla\delta\phi(\mathbf{r})$, we obtain another identity

$$\begin{aligned}\nabla\cdot(\delta\phi(\mathbf{r})\nabla\phi(\mathbf{r})) &= \nabla\delta\phi(\mathbf{r})\cdot\nabla\phi(\mathbf{r}) + \delta\phi(\mathbf{r})\nabla\cdot(\nabla\phi(\mathbf{r})) \\ &= \nabla\delta\phi(\mathbf{r})\cdot\nabla\phi(\mathbf{r}) + \delta\phi(\mathbf{r})\nabla^2\phi(\mathbf{r}),\end{aligned}$$

which when substituted to the functional change leads to

$$\begin{aligned}\delta F &= \int_V d^3\mathbf{r}\left[\nabla\cdot(\delta\phi(\mathbf{r})\nabla\phi(\mathbf{r})) - \delta\phi(\mathbf{r})\nabla^2\phi(\mathbf{r}) - 4\pi\rho(\mathbf{r})\delta\phi(\mathbf{r})\right] \\ &= \int_V d^3\mathbf{r}\left[\nabla\cdot(\delta\phi(\mathbf{r})\nabla\phi(\mathbf{r}))\right] - \int_V d^3\mathbf{r}\left[\delta\phi(\mathbf{r})\left(\nabla^2\phi(\mathbf{r}) + 4\pi\rho(\mathbf{r})\right)\right].\end{aligned}$$

The first integral in the result can be evaluated using Gauss's theorem

$$\int_V d^3\mathbf{r}(\nabla\cdot\mathbf{F}) = \oint_S d^2\mathbf{r}(\mathbf{F}\cdot\mathbf{n}), \tag{A.5.4}$$

where the left side is the volume integral and the right one is the surface integral over volume V boundary. Thus

$$\int_V d^3\mathbf{r}\left[\nabla\cdot(\delta\phi(\mathbf{r})\nabla\phi(\mathbf{r}))\right] = \oint_S d^2\mathbf{r}\left[\delta\phi(\mathbf{r})\nabla\phi(\mathbf{r})\right]\cdot\mathbf{n}.$$

Owing to the fact that over the surface S $\delta\phi(\mathbf{r})$ is zero, the integral is equal to zero too.